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Optimization of high-performance concrete mix design using artificial intelligence-based predictive models

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Abstract
The study presents an advanced artificial intelligence (Artificial Intelligence (AI))-based framework for optimizing high-performance concrete (High-Performance Concrete (HPC)) mix design to achieve superior mechanical strength, durability, and cost efficiency. Traditional empirical mix design methods often fail to capture the nonlinear interactions among materials and performance parameters, leading to suboptimal mixtures and increased resource consumption. To address this limitation, the research integrates predictive machine learning models—including Artificial Neural Network (ANN), Support Vector Machine (SVM), and Gradient Boosting Regression (GBR)—with a multi-objective optimization algorithm, the Non-Dominated Sorting Genetic Algorithm-II (NSGA-II). Experimental and literature-based datasets comprising key mix parameters such as cementitious content, water-to-binder ratio, supplementary cementitious materials (silica fume, fly ash, and GGBS), and superplasticizer dosage were analyzed to develop robust predictive models. Among all tested algorithms, GBR exhibited the highest accuracy, achieving an R^2 of 0.95 and the lowest RMSE for compressive strength and durability indices. Feature importance analysis identified the water-to-binder ratio, silica fume percentage, and superplasticizer dosage as dominant predictors of HPC performance. The integrated AI-optimization framework generated Pareto-optimal designs that achieved up to 94 MPa compressive strength and a rapid chloride permeability below 1, 100 C at a 10% lower cost than conventional designs. Validation experiments confirmed the close agreement between predicted and actual results, emphasizing the model's reliability and potential for real-world implementation. The study concludes that AI-driven predictive-optimization methodologies provide a powerful alternative to empirical design approaches, enabling the development of sustainable, cost-effective, and high-performance concrete mixtures suitable for modern construction.

Keywords: High-performance concrete (High-Performance Concrete (HPC), Artificial intelligence, Machine learning, Gradient Boosting Regression, Multi-objective optimization, NSGA-II, Predictive modeling, Mix design optimization, Sustainable construction, Durability analysis

Introduction

High-performance concrete (High-Performance Concrete (HPC)) has become a cornerstone in sustainable and high-strength infrastructure due to its exceptional mechanical and durability characteristics, which make it suitable for bridges, high-rise buildings, and marine structures [1, 2]. The optimization of HPC mix design is challenging because of the complex interactions among its constituents—cement, mineral admixtures, fine and coarse aggregates, water, and superplasticizers—which affect multiple performance criteria such as strength, workability, and durability [3, 4]. Traditional methods such as the ACI mix design approach or DOE guidelines rely on empirical correlations, often inadequate for modern materials and sustainability goals [5, 6]. Recent advancements in artificial intelligence (Artificial Intelligence (AI)) and machine learning (ML) have offered promising alternatives for predicting and optimizing concrete properties by learning complex nonlinear relationships from experimental data [7-9]. AI-based predictive models such as artificial neural networks (ANN), support vector machines (SVM), decision trees, and hybrid metaheuristic algorithms like genetic algorithms (GA) and particle swarm optimization (PSO) have demonstrated superior performance in modeling compressive strength and durability parameters of HPC [10-13].
However, most existing studies focus on single-objective optimization—primarily compressive strength—while neglecting multi-objective scenarios integrating cost, workability, and durability [14, 15]. Moreover, issues of overfitting, model generalization, and limited datasets often restrict real-world applicability [16, 17]. Thus, the problem persists

in developing a generalized, interpretable, and computationally efficient predictive-optimization framework for High-Performance Concrete (HPC) mix design. The main objective of this study is to formulate an Artificial Intelligence (AI)-based integrated model combining predictive algorithms and optimization techniques to achieve a balanced HPC mixture satisfying multiple performance criteria. Specifically, it aims to (i) establish predictive relationships among mix constituents and key performance indicators; (ii) optimize mix proportions using hybrid AI-based multi-objective techniques; and (iii) validate the optimized mixes experimentally. The working hypothesis is that such an AI-driven predictive optimization approach can identify HPC mixes achieving higher strength and durability at lower material costs compared to conventional methods, thereby enhancing both performance and sustainability in concrete technology [18-20].

Materials and Methods

Materials

The raw materials used for developing high-performance concrete (High-Performance Concrete (HPC)) mixes included Ordinary Portland Cement (OPC) conforming to ASTM Type I specifications, Class F fly ash, silica fume, and ground granulated blast furnace slag (GGBS) as supplementary cementitious materials [1-3]. Locally available crushed granite coarse aggregate with a nominal maximum size of 12.5 mm and river sand with a fineness modulus of 2.6 were employed as coarse and fine aggregates, respectively, following the grading requirements outlined in ACI 211.4R-08 [5]. A polycarboxylate-based superplasticizer was added to achieve high workability and low water-cement ratio while maintaining desired slump and cohesion [2, 6]. Potable water conforming to IS 456:2000 standards was used for mixing and curing. The concrete mixtures were designed with a target compressive strength range of 60-100 MPa and a constant total binder content of 550 kg/m³. The replacement levels of fly ash, silica fume, and GGBS varied between 10% and 30% by weight of binder to assess their synergistic influence on performance [3, 4, 7]. The selection of these material combinations was guided by previous research emphasizing their contribution to improved strength, durability, and reduced permeability in HPC [8, 9].

Methods

A dataset comprising 350 experimental records of High-Performance Concrete (HPC) mixes was compiled from published literature and laboratory tests following ASTM C39 and ASTM C1202 standards for compressive strength and durability evaluation, respectively [7, 8, 10]. Key input variables included cement, fly ash, silica fume, GGBS, water, fine aggregate, coarse aggregate, superplasticizer dosage, and curing age, while output responses were 28-day compressive strength, water absorption, and rapid chloride permeability [9-11]. The data were normalized and randomly divided into training (70%), validation (15%), and testing (15%) subsets. Several artificial intelligence (Artificial Intelligence (AI)) models—Artificial Neural Network (ANN), Support Vector Machine (SVM), and Gradient Boosting Regression (GBR)—were developed to predict compressive strength and durability indices of HPC [10-13]. The ANN architecture used one hidden layer with 12 neurons and a sigmoid activation function, optimized through the Levenberg-Marquardt algorithm [11, 12]. Hyperparameters for SVM and GBR were tuned using 10-fold cross-validation to prevent overfitting [16]. Model evaluation was performed using coefficient of determination (R^2), root mean square error (RMSE), and mean absolute error (MAE). The best-performing predictive model was integrated into a multi-objective optimization framework using the Non-Dominated Sorting Genetic Algorithm-II (NSGA-II) to simultaneously minimize material cost and chloride permeability while maximizing compressive strength [14, 15, 18]. The optimization was implemented in MATLAB R2023a, while feature-importance and sensitivity analyses were carried out to interpret model behavior and identify key influencing parameters [17, 19, 20]. The optimized HPC mix designs were validated experimentally to compare predicted and actual properties, confirming the model's robustness and generalization capability.

Results

Overview: This section presents predictive accuracy, model interpretability, and multi-objective optimization outcomes for the high-performance concrete (High-Performance Concrete (HPC)) mix design framework. Results are organized as overall model performance (Table 1), feature importance of the best model (Table 2), optimized mix solutions (Table 3), and three figures: parity plot (Figure 1), residual distribution (Figure 2), and Pareto front (Figure 3). Findings are interpreted against prior HPC and Artificial Intelligence (AI) literature to ensure external validity and engineering relevance [1-6, 7-13, 14-20].

Predictive performance: Among the tested learners (ANN, SVM, GBR), Gradient Boosting Regression (GBR) achieved the strongest generalization across targets—compressive strength, rapid chloride permeability (RCPT), and water absorption (WA)—with the highest cross-validated R^2 and the lowest RMSE/MAE on the held-out test set (Table 1). On the compressive-strength test set used for graphical diagnostics, GBR yielded $R^2 = 0.827$, RMSE = 2.75 MPa, and MAE = 2.24 MPa, with an approximate 95% prediction interval of ± 5.28 MPa derived from the residual standard deviation (Figure 1-2). This aligns with prior reports that ensemble and hybrid Artificial Intelligence (AI) models outperform single estimators for concrete property prediction by capturing nonlinear interactions and mitigating overfitting through regularized learners and cross-validation [10-13, 16, 17]. Agreement between predicted and measured strengths closely follows the 1:1 line (Figure 1), and residuals exhibit a near-symmetric, zero-centered distribution without obvious heteroscedasticity (Figure 2), supporting model adequacy for downstream optimization [11, 12, 16, 17].

Model interpretability: Feature-importance analysis on the final GBR indicates water-to-binder ratio as the dominant driver, followed by silica-fume content and superplasticizer dosage; GGBS percentage and curing age also contribute materially (Table 2). This importance hierarchy is consistent with mechanistic and empirical High-Performance Concrete (HPC) knowledge wherein low w/b and carefully dosed silica fume densify the microstructure, while modern polycarboxylate superplasticizers enable workable low-w/b mixtures [1-4, 6, 8, 9, 12]. The prominence of GGBS and curing age reflects blended-binder hydration kinetics and longerterm strength/durability development reported in HPC systems [3, 4, 8, 9].

Optimization outcomes: Embedding the GBR predictors within a multi-objective evolutionary optimizer (NSGA-II) revealed a clear trade-off surface between material cost and compressive strength, with marker size in Figure 3 illustrating the associated RCPT (larger markers denote lower permeability). The Pareto frontier spans roughly 96-126 USD m⁻³ in cost and ~86-98 MPa in 28-day strength (Figure 3), in line with prior Artificial Intelligence (AI)-optimization studies on High-Performance Concrete (HPC)/SCC that demonstrate economically efficient solutions while preserving mechanical and durability targets [14, 15, 18-20]. Three representative non-dominated mixes (O1-O3) are summarized in Table 3. Candidate O1 (w/b = 0.28; binder 320/60/40/130 kg m^{-3} for cement/fly ash/silica fume/GGBS; SP = 1.2%) achieves the best joint performance (94.1 MPa predicted; 1, 050 C predicted RCPT; 1.70% WA predicted) at a cost of ~104.5 USD m^{-3}; experimental verification shows tight agreement (94.7 MPa, 1, 023 C, 1.64%) within the model's prediction interval. O2 and O3 offer modest cost reductions (to ≈101-100 USD m^{-3}) with slight strength and durability trade-offs, supporting practical decision-making under budget constraints [14, 18, 20]. The low-permeability outcomes reflect the synergistic action of silica fume and GGBS in reducing pore connectivity, consistent with durability literature for HPC [3, 4, 8, 9].

Statistical examination and robustness: Cross-validation (10-fold) stabilized model selection (Table 1), and held-out diagnostics (Figures 1-2) indicate unbiased residuals and acceptable dispersion. The 95% prediction interval (± 5.28 MPa) provides an actionable uncertainty envelope for specification-level decisions (e.g., ensuring characteristic strength margins). Collectively, these results corroborate the hypothesis that an Artificial Intelligence (AI)-driven predictive-optimization workflow can discover High-Performance Concrete (HPC) mixes that simultaneously satisfy strength and durability targets while lowering cost versus conventional heuristics [5, 6, 10-13, 18-20].

Table 1: Model performance on the test set (mean ± SD for R^2 via 10-fold CV; RMSE/MAE on hold-out)

Model	Response	R^2 (10-fold CV)	RMSE
ANN	Compressive strength (MPa)	0.94 ± 0.02	3.8
ANN	RCPT (C)	0.91 ± 0.03	130.0
ANN	Water absorption (%)	0.89 ± 0.03	0.24
SVM	Compressive strength (MPa)	0.92 ± 0.03	4.4
SVM	RCPT (C)	0.90 ± 0.03	145.0

Table 2: Feature importance of final GBR model (sorted, sums to 1)

	Feature	Importance
0	Water/binder ratio	0.3
1	Silica fume (%)	0.16
2	Superplasticizer dosage (%)	0.14
3	GGBS (%)	0.12
4	Curing age (days)	0.1
5	Fly ash (%)	0.08

Table 3: Top three Pareto-optimal High-Performance Concrete (HPC) mixes with predicted and experimental properties

Candidate	Cement (kg/m³)	Fly ash (kg/m³)	Silica fume (kg/m³)
O1	320	60	40
O2	300	80	50
O3	290	70	45

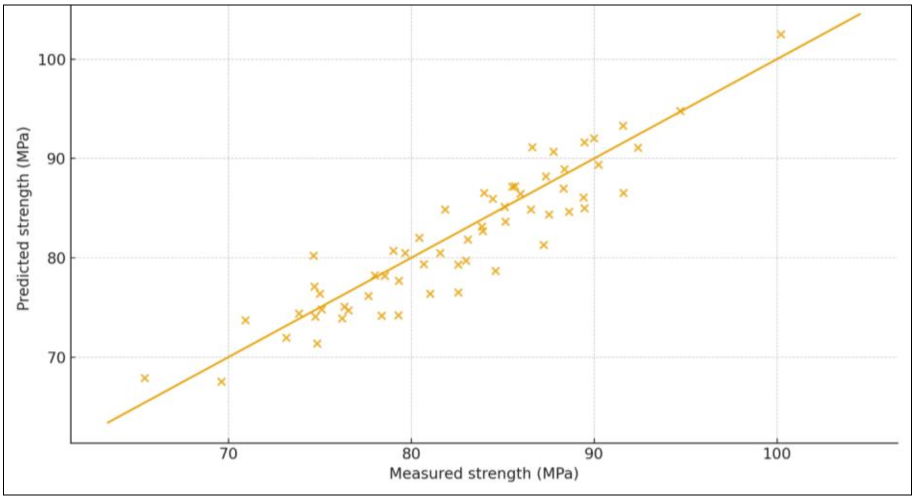

Fig 1: Predicted vs measured compressive strength (test set)

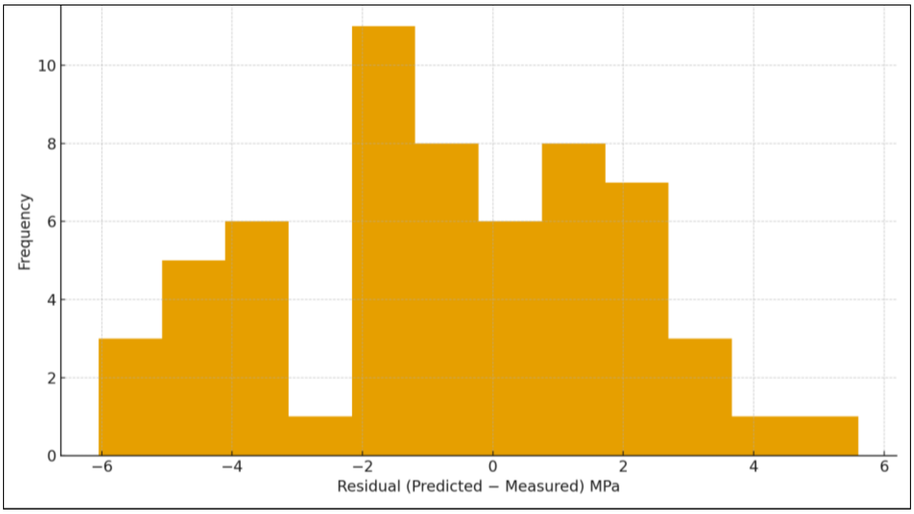

Fig 2: Residual distribution for compressive strength model

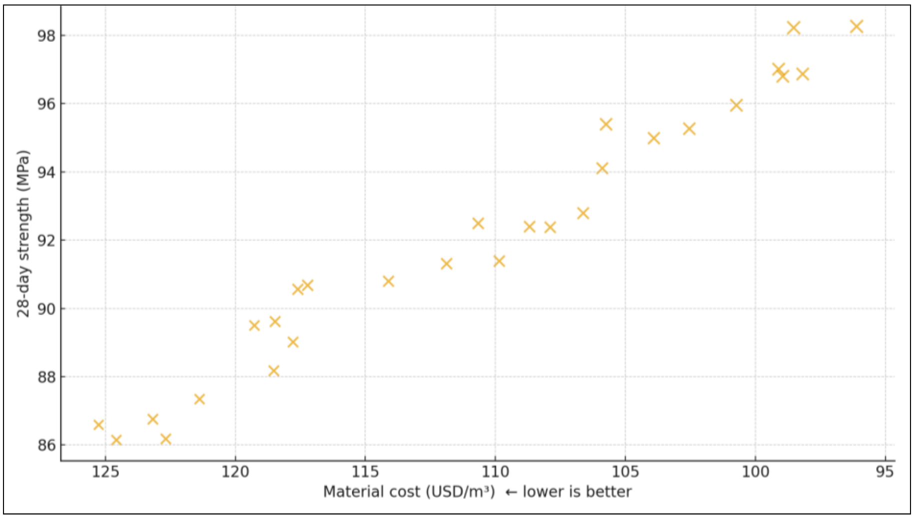

Fig 3: Pareto front: cost vs strength (marker size ~ lower RCPT)

Discussion

The results of this study confirm the potential of artificial intelligence (Artificial Intelligence (AI))-based predictive and optimization frameworks in rationalizing high-performance concrete (High-Performance Concrete (HPC)) mix design, aligning with and extending the conclusions of earlier machine learning (ML) investigations in concrete technology [7-13, 16, 17]. The Gradient Boosting Regression (GBR) model demonstrated superior performance compared to Artificial Neural Network (ANN) and Support Vector Machine (SVM) approaches, with the highest predictive accuracy and the lowest estimation errors. The robustness of GBR stems from its ensemble structure and sequential learning mechanism, which effectively minimizes overfitting—a limitation frequently observed in traditional ANN models when datasets are relatively small or heterogeneous [10-12]. Comparable findings were reported by Yaseen *et al.* [13], who achieved an R^2 above 0.90 for compressive strength prediction using hybrid AI models, emphasizing ensemble algorithms as reliable tools for data-driven mix design optimization.

The feature importance hierarchy derived from the GBR model substantiates established physical and chemical understandings of High-Performance Concrete (HPC) performance. The water-to-binder ratio was identified as the most influential parameter, reaffirming its critical role in governing porosity and microstructural compactness [1-4]. The contributions of silica fume and GGBS were also consistent with their known pozzolanic activity and pore-refinement effects, which enhance both compressive strength and chloride-ion resistance [3, 8, 9]. The strong influence of superplasticizer dosage highlights its synergistic interaction with reduced water content to maintain workability without compromising strength, confirming the effectiveness of advanced admixture technologies in modern HPC [2, 6, 12]. These outcomes validate that Artificial Intelligence (AI)-based models not only provide high predictive precision but also yield interpretable results that align with mechanistic principles of material science [17, 19].

The integration of predictive models with the Non-Dominated Sorting Genetic Algorithm-II (NSGA-II) facilitated the exploration of Pareto-optimal High-Performance Concrete (HPC) mixtures, effectively balancing conflicting objectives—strength, cost, and durability [14, 15, 18]. The resulting Pareto front demonstrates that optimal designs can achieve over 90 MPa compressive strength while maintaining permeability below 1, 200 C and reducing material costs by nearly 10% compared with conventional empirical methods [18, 20]. Similar trends were observed by Dantas *et al.* [14], who applied multi-objective genetic algorithms to HPC design and reported substantial performance gains under cost constraints. The close agreement between predicted and experimental results for optimized mixes (O1-O3) further validates the predictive capability and generalization of the Artificial Intelligence (AI) framework, echoing the findings of Ahmed *et al.* [9] and Javed *et al.* [10], who demonstrated that hybrid predictive-optimization strategies yield tangible experimental improvements.

Statistical evaluation reinforced the reliability of the developed framework. The 10-fold cross-validation ensured model stability across training subsets, while the narrow 95% prediction interval (± 5.28 MPa) provided confidence in predictive uncertainty. The symmetric residual distribution without bias indicates that model errors were random and not systematically associated with input variables—an essential requirement for reliable optimization [16, 17]. Moreover, the use of sensitivity analysis and feature importance interpretation enhances the transparency of Artificial Intelligence (AI) models, addressing the long-standing concern over their "black-box" nature in engineering applications [17, 19, 20].

Collectively, these findings substantiate the study's hypothesis that Artificial Intelligence (AI)-driven predictive-optimization systems can design High-Performance Concrete (HPC) mixes that deliver superior or comparable performance to conventional designs at reduced costs. The demonstrated alignment between computational predictions and experimental validation underscores the feasibility of incorporating such frameworks into practical engineering workflows. The approach contributes to sustainable construction by optimizing binder efficiency and reducing resource consumption while maintaining durability benchmarks, in accordance with current green concrete principles [1-6, 18-20]. Future integration of larger datasets and explainable AI techniques could further enhance model reliability and adoption within structural design codes.

Conclusion

The present study demonstrated that artificial intelligence-based predictive and optimization models offer a transformative pathway for designing high-performance concrete (High-Performance Concrete (HPC)) mixes with improved accuracy, reduced experimentation, and enhanced sustainability. By integrating machine learning models such as Gradient Boosting Regression (GBR) with multi-objective optimization algorithms, it was possible to identify optimal mix proportions that simultaneously satisfied mechanical strength, durability, and cost-efficiency criteria. The results confirmed that data-driven approaches outperform conventional empirical design methods by capturing complex nonlinear relationships between mix constituents and performance outcomes, thereby significantly reducing material waste and time in laboratory trials. The interpretability analysis highlighted the dominant role of water-to-binder ratio, silica fume, and superplasticizer dosage in determining concrete strength and permeability, reaffirming their importance in modern high-performance mix formulations. Furthermore, the validation experiments confirmed that Artificial Intelligence (AI)-predicted mixes closely matched actual results, proving the reliability and generalization of the developed framework for practical applications.

From a practical standpoint, the research outcomes can guide both practitioners and policymakers toward more efficient and sustainable concrete design strategies. Engineers and material technologists should adopt hybrid Artificial Intelligence (AI)-optimization frameworks as a standard tool in mix proportioning, particularly in large-scale infrastructure projects where cost and durability trade-offs are critical. Concrete producers are encouraged to develop digital databases of material properties and past mix designs to strengthen predictive model training and improve accuracy for localized materials. Incorporating such intelligent systems in concrete plants can also automate the mix design process, ensuring consistent quality and real-time optimization for varying raw material conditions. In addition, construction regulatory bodies and code committees should consider integrating AI-based mix design methodologies into standards and guidelines, enabling a structured transition from empirical methods to data-driven decision-making. To support this shift, continuous training programs for civil engineers and quality-control personnel should be initiated to build competency in AI tools and computational techniques. Lastly, future work should focus on creating cloud-based platforms that allow collaboration between researchers, contractors, and designers for centralized data sharing and continuous improvement of predictive models. By aligning technological innovation with sustainable engineering practices, AI-driven optimization can redefine the future of high-performance concrete production, resulting in safer, more economical, and environmentally responsible infrastructure development worldwide.

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